

chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

Match level :

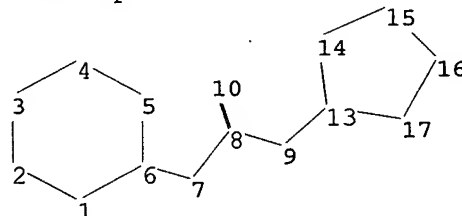
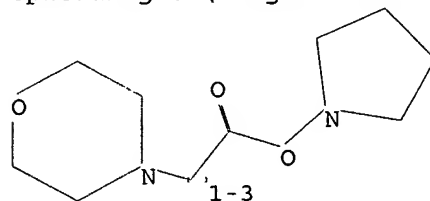
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\Stnexp\Queries\10765267pt2.str



chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6 13 14 15 16 17

chain bonds :

6-7 7-8 8-9 8-10 9-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 8-9 8-10 9-13 13-14 13-17 14-15 15-16 16-17

exact bonds :

7-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

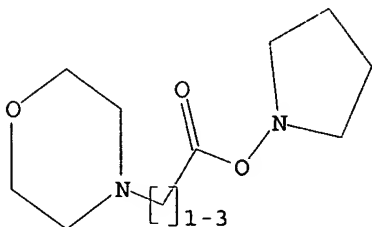
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L2 STRUCTURE UPLOADED

=> d 12

L2 HAS NO ANSWERS

L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 12

SAMPLE SEARCH INITIATED 15:00:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8 TO 329

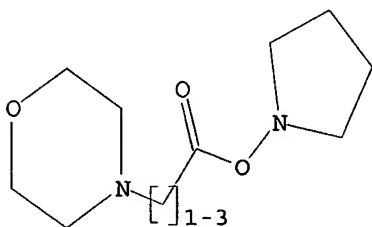
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:00:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

Ngrazier 10765267

PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:00:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 172 TO ITERATE

100.0% PROCESSED 172 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 163.05 163.26

FILE 'HCAPLUS' ENTERED AT 15:00:53 ON 08 SEP 2005
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FILE COVERS 1907 - 8 Sep 2005 VOL 143 ISS 11
FILE LAST UPDATED: 7 Sep 2005 (20050907/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l5
L6 4 L5
=> d ed abs ibib hitstr 1-4

L6 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Oct 2004

AB Provided is a method for characterizing a mol. by mass spectrometry, which mol. comprises one or more free amino groups, which method comprises: (a) reacting one or more free amino groups in the mol. with a mass tag reagent comprising a reactive functionality capable of reacting with an amino group, and a tertiary amino group linked to the reactive functionality; and (b) characterizing the mol. by mass spectrometry.

ACCESSION NUMBER: 2004:824132 HCAPLUS

DOCUMENT NUMBER: 141:310231

TITLE: Mass labels

INVENTOR(S): Hamon, Christian; Kuhn, Karsten; Thompson, Andrew; Reuschling, Dieter; Schaefer, Juergen

PATENT ASSIGNEE(S): Xzillion G.m.b.H. & Co. K.-G., Germany; Proteome Sciences PLC

SOURCE: PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004086050	A2	20041007	WO 2004-GB1167	20040318
WO 2004086050	A3	20041229		
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW</p> <p>RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				

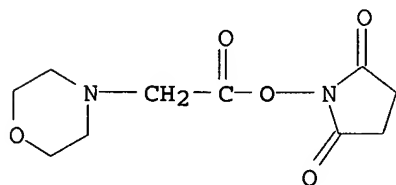
PRIORITY APPLN. INFO.: GB 2003-6756 A 20030324

IT 741683-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (mass labels)

RN 741683-76-1 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy] - (9CI) (CA INDEX NAME)



L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Aug 2004

AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

ACCESSION NUMBER: 2004:681717 HCAPLUS

DOCUMENT NUMBER: 141:202794

TITLE: Methods, mixtures, kits and compositions pertaining to analyte determination

INVENTOR(S): Pappin, Darryl J. C.; Bartlet-Jones, Michael

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004070352	A2	20040819	WO 2004-US2077	20040127
<p>W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI</p> <p>RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG</p>				
CA 2488584	AA	20040819	CA 2004-2488584	20040127
US 2004219685	A1	20041104	US 2004-765264	20040127
US 2004220412	A1	20041104	US 2004-765267	20040127
US 2004219686	A1	20041104	US 2004-765458	20040127
PRIORITY APPLN. INFO.:			US 2003-443612P	P 20030130
			WO 2004-US2077	W 20040127

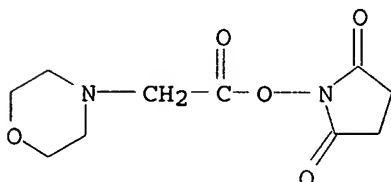
App 1

IT 741683-76-1P 741683-77-2P 741683-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(methods, mixts., kits and compns. pertaining to analyte determination)

RN 741683-76-1 HCAPLUS

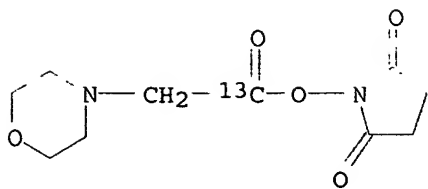
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME)



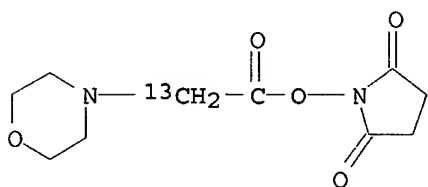
RN 741683-77-2 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)

Ngrazier 10765267



RN 741683-78-3 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2- ^{13}C)oxy] - (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 30 May 1997

AB The title polymers having a single reactive moiety at one end of the polymer chain have the following structure R-Z-X-Y (R = N-acryloylmorpholine residue with d.p. 6-280, which yields number-average mol. weight 1000-40,000; Z-X-Y = polymer capping moiety; X = saturated residue of linear or branched aliphatic series CrH_{2r} , $r' = 1-12$; Y = reactive moiety, such as -OH, -CO₂H, or -NH₂; Z = moiety that readily reacts to cap a polymer free radical, e.g., S). The monofunctional polymer is a suitable alternative to monofunctional PEG for modification of substances having biol. and biotech. applications.

ACCESSION NUMBER: 1997:341994 HCAPLUS

DOCUMENT NUMBER: 127:34643

TITLE: Polymers of N-acryloylmorpholine derivative activated at one end and conjugates with bioactive materials and surfaces

INVENTOR(S): Veronese, Francesco M.; Schiavon, Oddone; Caliceti, Paolo; Sartore, Luciana; Ranucci, Elisabetta; Ferruti, Paolo

PATENT ASSIGNEE(S): Consiglio Nazionale Delle Ricerche, Italy

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5629384	A	19970513	US 1994-243869	19940517
US 5631322	A	19970520	US 1995-475177	19950607
PRIORITY APPLN. INFO.:			US 1994-243869	A3 19940517

IT 190727-27-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); PRP (Properties); BIOL (Biological study); PREP (Preparation)

(polymers of N-acryloylmorpholine derivative activated at one end and conjugates with bioactive materials and surfaces)

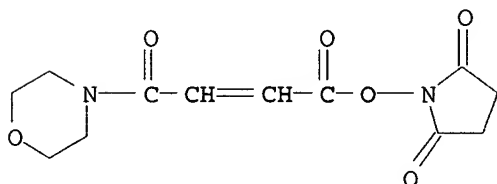
RN 190727-27-6 HCAPLUS

CN Morpholine, 4-[4-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1,4-dioxo-2-butenyl]-, homopolymer (9CI) (CA INDEX NAME)

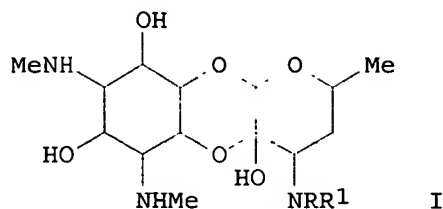
CM 1

CRN 190727-26-5

CMF C12 H14 N2 O6



L6 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 ED Entered STN: 12 May 1984
 GI



AB Spectinomycylamines I [R = alkyl, optionally substituted CH₂Ph, cyclohexyl, oxoalkyl, hydroxyalkyl, optionally substituted benzoylalkyl, acyl, aminoalkyl, amino(hydroxy)alkyl, amino(oxo)alkyl, carbamoylphenyl; R₁ = H, Me] were prepared and showed bactericidal activity. Thus 6,8-bis(benzyloxycarbonyl)spectinomycin was treated with Me₂CHNH₂ and NaB(CN)H₃, and the product was subjected to hydrogenolysis to give I (R = CHMe₂, R₁ = H), which had a ED₅₀ against Escherichia coli ATCC 11775 of 9 mg/kg s.c. in mice.

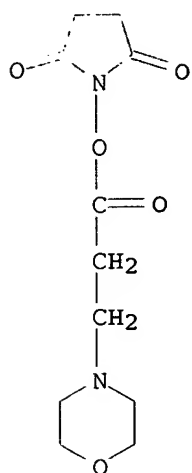
ACCESSION NUMBER: 1980:639849 HCAPLUS
 DOCUMENT NUMBER: 93:239849
 TITLE: Spectinomycylamines and pharmaceutical compositions containing them
 INVENTOR(S): Woitun, Eberhard; Maier, Roland; Reuter, Wolfgang; Wetzell, Bernd; Goeth, Hanns; Lechner, Uwe; Werner, Uwe
 PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 102 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2851953	A1	19800619	DE 1978-2851953	19781201
PRIORITY APPLN. INFO.:			DE 1978-2851953	A 19781201

IT 75727-76-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (N-acylation of bis(benzyloxycarbonyl)spectinomycylamine by)

RN 75727-76-3 HCAPLUS
 CN 2,5-Pyrrolidinedione, 1-[3-(4-morpholinyl)-1-oxopropoxy] - (9CI) (CA INDEX NAME)

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=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

24.66

187.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.92

-2.92

STN INTERNATIONAL LOGOFF AT 15:01:51 ON 08 SEP 2005

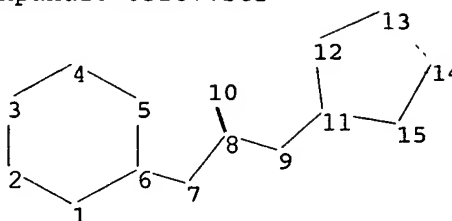
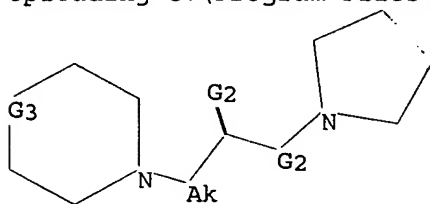
Ngrazier 10765267expand

=> screen 2039

L1 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\expand10765267.str



chain nodes :

7 8 9 10

ring nodes :

1 2 3 4 5 6 11 12 13 14 15

chain bonds :

6-7 7-8 8-9 8-10 9-11

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-10 9-11 11-12 11-15 12-13 13-14 14-15

isolated ring systems :

containing 1 : 11 :

G1:C,N

G2:O,S

G3:C,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom

L2 STRUCTURE UPLOADED

=> que L2 AND L1

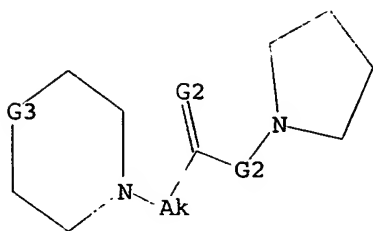
L3 QUE L2 AND L1

=> d l3

L3 HAS NO ANSWERS

L1 SCR 2039

L2 STR



G1 C,N

G2 O,S

G3 C,O,N

Structure attributes must be viewed using STN Express query preparation.

L3 QUE L2 AND L1

=> s l3

SAMPLE SEARCH INITIATED 15:50:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L2 AND L1

=> s l3 full

FULL SEARCH INITIATED 15:50:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

L5 9 SEA SSS FUL L2 AND L1

=> fil hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.77	164.98

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FILE LAST UPDATED: 7 Sep 2005 (20050907/ED)

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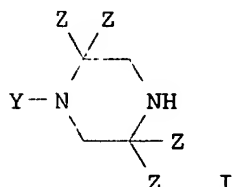
=> s l5

L6 7 L5

=> d ed abs ibib hitstr 1-7

L6 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 08 Jul 2005
GI

EFO 1/30/03



AB Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of ¹³C and/or ¹⁵N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-¹³C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-¹³C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-¹³C.

ACCESSION NUMBER: 2005:592130 HCAPLUS
DOCUMENT NUMBER: 143:115574
TITLE: Preparation of isotopically enriched N-substituted piperazines
INVENTOR(S): Pappin, Darryl J. C.; Pillai, Sasi; Coull, James M.
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ. 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

Inv #1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2005148773	A1	20050707	US 2004-751388	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

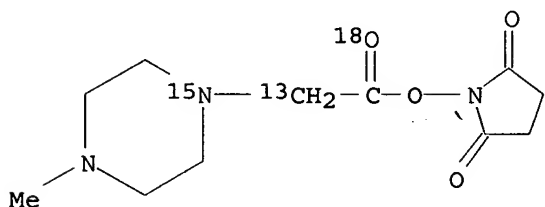
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PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

IT 856188-20-0P
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

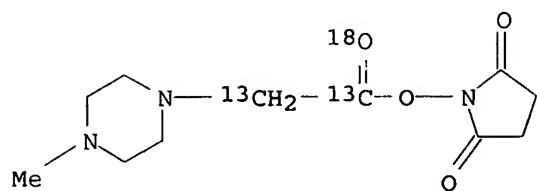
RN 856188-20-0 HCAPLUS
 CN 2,5-Pyrrolidinedione, 1-[[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

IT 856188-16-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856188-16-4 HCAPLUS
 CN 2,5-Pyrrolidinedione, 1-[[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



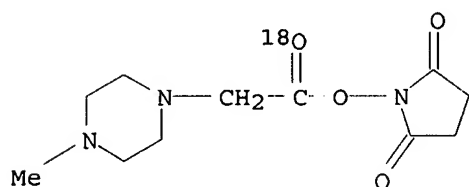
● 2 HCl

IT 856187-87-6P

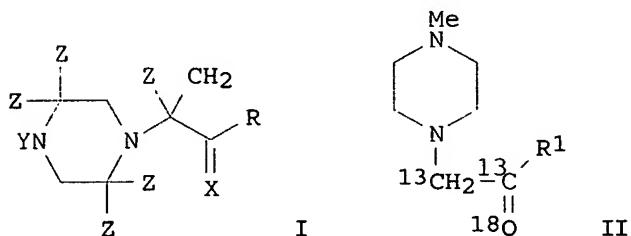
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[4-methyl-1-piperazinyl]acetyl- ^{18}O]oxy] - (9CI)
(CA INDEX NAME)



L6 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
 ED Entered STN: 08 Jul 2005
 GI



AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

ACCESSION NUMBER: 2005:592129 HCAPLUS

DOCUMENT NUMBER: 143:97398

TITLE: Preparation of active esters of N-substituted piperazine acetic acids, including isotopically enriched versions

INVENTOR(S): Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.

PATENT ASSIGNEE(S): Applera Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148771	A1	20050707	US 2004-751354	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:	US 2004-751353	A	20040105
	US 2004-751354	A	20040105
	US 2004-751387	A	20040105
	US 2004-751388	A	20040105
	US 2004-822639	A	20040412
	US 2004-852730	A	20040524

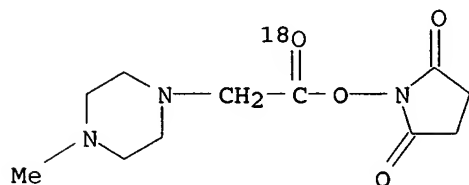
IT 856187-87-6P 856188-16-4P 856188-20-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

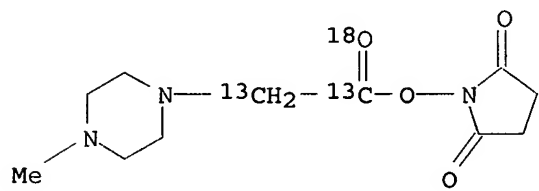
RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl) acetyl-18O]oxy]- (9CI)
(CA INDEX NAME)



RN 856188-16-4 HCAPLUS

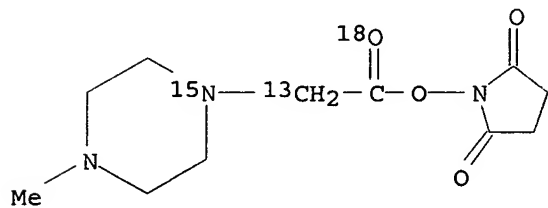
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl) acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N) acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

L6 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

ACCESSION NUMBER: 2005:592027 HCAPLUS

DOCUMENT NUMBER: 143:93642

TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom

INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.

PATENT ASSIGNEE(S): Applera Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

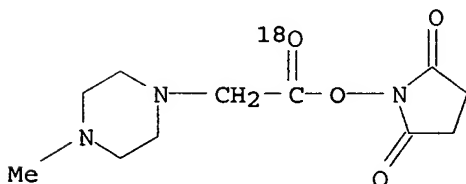
PRIORITY APPLN. INFO.: US 2004-751353 A2 20040105
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A2 20040412
US 2004-852730 A 20040524

IT 856187-87-6P 856188-16-4P 856188-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI)
(CA INDEX NAME)

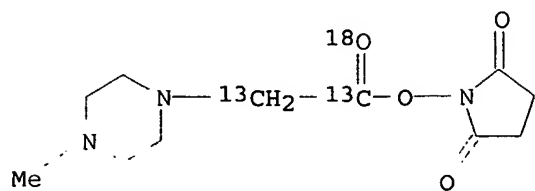


RN 856188-16-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-,

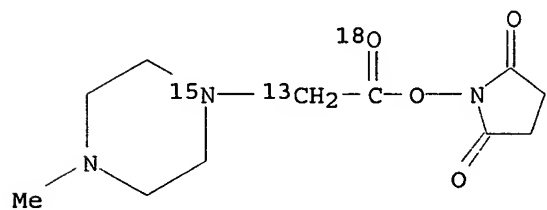
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dihydrochloride (9CI) (CA INDEX NAME)



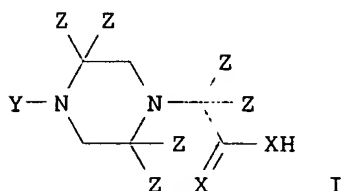
●2 HCl

RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[4-methyl-1-piperazinyl-1-15N]acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L6 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
 ED Entered STN: 08 Jul 2005
 GI



AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

ACCESSION NUMBER:	2005:588426 HCAPLUS
DOCUMENT NUMBER:	143:115568
TITLE:	Preparation of isotopically enriched N-substituted piperazine-1-acetic acids
INVENTOR(S):	Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
PATENT ASSIGNEE(S):	Applera Corp., USA
SOURCE:	U.S. Pat. Appl. Publ., 29 pp. CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	6
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148774	A1	20050707	US 2004-751387	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

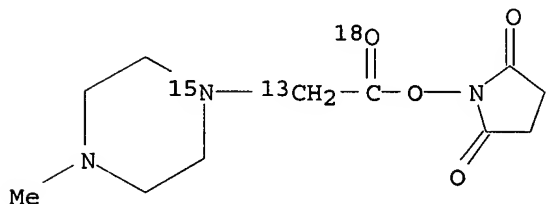
PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

IT **856188-20-0P**
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[4-methyl-1-piperazinyl-1-15N]acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

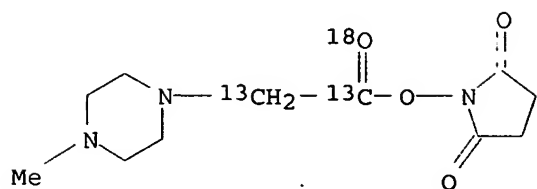


● 2 HCl

IT **856188-16-4P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

RN 856188-16-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[4-methyl-1-piperazinyl]acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



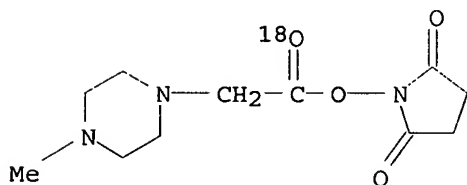
● 2 HCl

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazine-1-acetic
acids as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[4-methyl-1-piperazinyl]acetyl- ^{18}O]oxy]- (9CI)
(CA INDEX NAME)



L6 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to isobarically labeled analytes and fragment ions thereof.

ACCESSION NUMBER: 2005:588349 HCAPLUS

DOCUMENT NUMBER: 143:112150

TITLE: Isobarically labeled analytes and fragment ions derived therefrom

INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148087	A1	20050707	US 2004-852730	20040524
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
WO 2005068446	A1	20050728	WO 2005-US223	20050105

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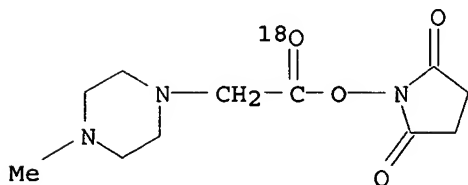
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PRIORITY APPLN. INFO.:
US 2004-751353 A2 20040105
US 2004-822639 A2 20040412
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-852730 A 20040524

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[4-methyl-1-piperazinyl)acetyl-18O]oxy] - (9CI)
(CA INDEX NAME)

L6 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2005

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

ACCESSION NUMBER: 2005:588336 HCAPLUS

DOCUMENT NUMBER: 143:93635

TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom

INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 6

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

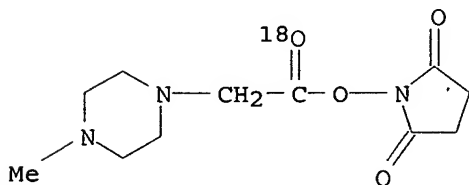
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US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A2 20040412
US 2004-852730 A 20040524

IT 856187-87-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[(4-methyl-1-piperazinyl)acetyl-18O]oxy] - (9CI)
(CA INDEX NAME)

L6 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Aug 2004

AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

ACCESSION NUMBER: 2004:681717 HCAPLUS

DOCUMENT NUMBER: 141:202794

TITLE: Methods, mixtures, kits and compositions pertaining to analyte determination

INVENTOR(S): Pappin, Darryl J. C.; Bartlet-Jones, Michael

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: PCT Int. Appl., 105 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004070352	A2	20040819	WO 2004-US2077	20040127
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RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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US 2004219685	A1	20041104	US 2004-765264	20040127
US 2004220412	A1	20041104	US 2004-765267	20040127
US 2004219686	A1	20041104	US 2004-765458	20040127
PRIORITY APPLN. INFO.:			US 2003-443612P	P 20030130
			WO 2004-US2077	W 20040127

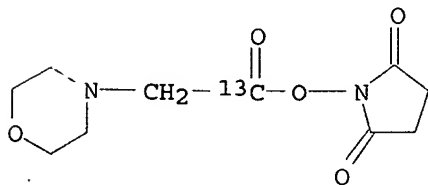
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741683-93-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(methods, mixts., kits and compns. pertaining to analyte determination)

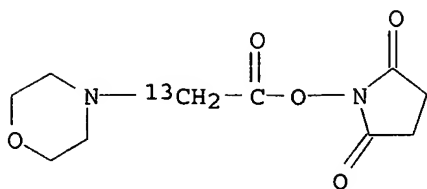
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CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)

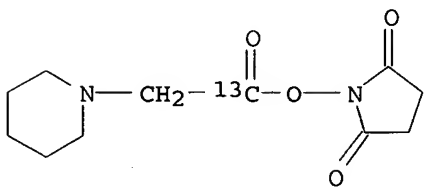


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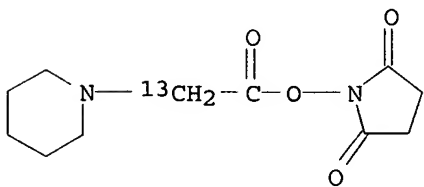
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RN 741683-86-3 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-1- ^{13}C)oxy]- (9CI) (CA INDEX NAME)



RN 741683-93-2 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-2- ^{13}C)oxy]- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

37.03

202.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-5.11

-5.11

STN INTERNATIONAL LOGOFF AT 15:51:21 ON 08 SEP 2005